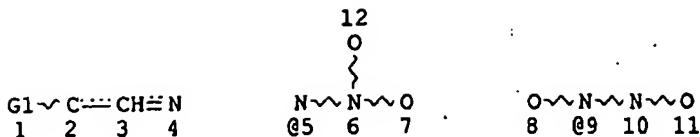


=> d que

L22 STR



VAR G1=5/9

NODE ATTRIBUTES:

NSPEC IS RC AT 2
 NSPEC IS RC AT 4
 CONNECT IS E2 RC AT 5
 CONNECT IS E3 RC AT 6
 CONNECT IS E1 RC AT 7
 CONNECT IS E1 RC AT 8
 CONNECT IS E3 RC AT 9
 CONNECT IS E2 RC AT 10
 CONNECT IS E1 RC AT 11
 CONNECT IS E1 RC AT 12
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L24 16 SEA FILE=REGISTRY SSS FUL L22
 L25 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L24

=> d ibib abs hitstr 125 1-6

L25 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 2001:502352 HCAPLUS
 DOCUMENT NUMBER: 135:256880
 TITLE: DFT studies for the substituent effect on the
 Diels-Alder reaction of 1,4-diaza-1,3-butadienes
 AUTHOR(S): Lee, Gab-Yong
 CORPORATE SOURCE: Department of Chemistry, Catholic University of Taegu,
 Kyongsan, 712-702, S. Korea
 SOURCE: Journal of the Korean Chemical Society (2001), 45(3),
 207-212
 CODEN: JKCSEZ; ISSN: 1017-2548
 PUBLISHER: Korean Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: Korean
 AB DFT calcns. have been performed on several substituted
 1,4-diaza-1,3-butadienes (1,4-DABs) with electron donating and withdrawing
 groups at the terminal two nitrogens to investigate the reactivity of
 Diels-Alder reaction with acrolein. The calcd. FMO (frontier MO) energies
 for the optimized 1,4-disubstituted-1,4-DABs have been used to explain
 both normal and inverse electron demand Diels-Alder reactions. It is
 shown that the electron donating and withdrawing substituents lead to the